

=> b hcaplus

FILE 'HCAPLUS' ENTERED AT 15:08:17 ON 19 NOV 2004

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 22

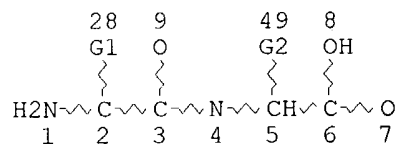
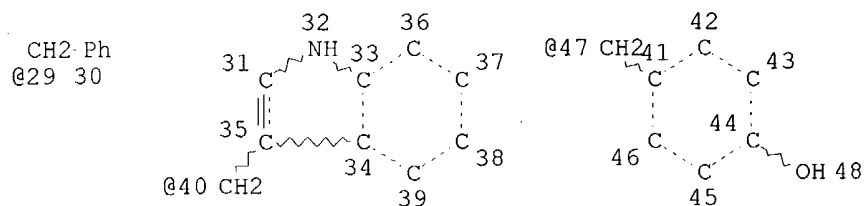
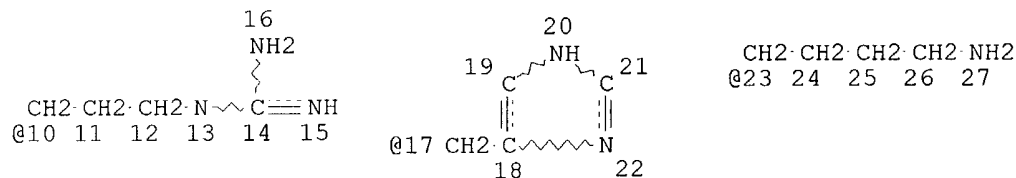
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que 114

L8 STR



VAR G1=10/17/23

VAR G2=29/40/47

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 7

CONNECT IS E1 RC AT 9

CONNECT IS X2 RC AT 19

CONNECT IS X2 RC AT 21

Searched by P. Ruppel

CONNECT IS X2 RC AT 31  
 CONNECT IS X3 RC AT 33  
 CONNECT IS X3 RC AT 34  
 CONNECT IS X3 RC AT 35  
 CONNECT IS X2 RC AT 36  
 CONNECT IS X2 RC AT 37  
 CONNECT IS X2 RC AT 38  
 CONNECT IS X2 RC AT 39  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE

L9 ( 77)SEA FILE=REGISTRY SSS FUL L8  
 L10 ( 412)SEA FILE=HCAPLUS ABB=ON PLU=ON L9  
 L11 ( 5334)SEA FILE=HCAPLUS ABB=ON PLU=ON TASTE+NT/CT  
 L12 ( 20583)SEA FILE=HCAPLUS ABB=ON PLU=ON FLAVOR+NT,OLD/CT  
 L13 ( 54057)SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR L12 OR FLAVOUR?/OBI OR  
 FLAVOR?/OBI OR TASTE/OBI OR PALATABIL?/OBI  
 L14 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND L13

=> d ibib abs hitstr l14 1-10

L14 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2003:259690 HCAPLUS  
 DOCUMENT NUMBER: 138:270653  
 TITLE: **Flavor**-active peptides from cocoa beans  
 INVENTOR(S): Kochhar, Sunil; Hansen, Carl Erik; Juillerat, Marcel  
 Alexandre  
 PATENT ASSIGNEE(S): Societe Des Produits Nestle S.A., Switz.  
 SOURCE: Eur. Pat. Appl., 14 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1297753	A1	20030402	EP 2001-123585	20011001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
WO 2003028479	A1	20030410	WO 2002-EP10031	20020906
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004224077	A1	20041111	US 2004-812088	20040330

## PRIORITY APPLN. INFO.:

EP 2001-123585 A 20011001  
WO 2002-EP10031 A1 20020906

AB The present invention pertains to specific peptides obtainable from cocoa beans and giving rise to a particular and distinct flavor when subjected to a Maillard reaction with reducing sugars. In particular the present invention pertains to the use of said specific peptides for the preparation of a chocolate flavor, specifically a cocoa and a caramel flavor, a floral or specifically, a bonbon flavor, a bready flavor, a roasted flavor and a meat flavor.

IT 2047-13-4 6235-35-4, Lys-Phe

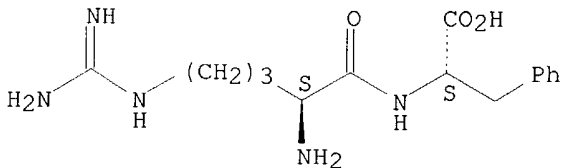
RL: FFD (Food or feed use); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(flavor-active peptides from cocoa beans)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

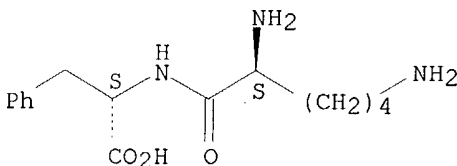
Absolute stereochemistry.



RN 6235-35-4 HCAPLUS

CN L-Phenylalanine, L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



## REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:193419 HCAPLUS

DOCUMENT NUMBER: 139:53285

TITLE: Relative hydrophobicity of di- to hexapeptides as  
measured by aqueous two-phase partitioning

AUTHOR(S): Gulyaeva, N.; Zaslavsky, A.; Chait, A.; Zaslavsky, B.

CORPORATE SOURCE: Analiza, Inc., Cleveland, OH, 44128, USA

SOURCE: Journal of Peptide Research (2003), 61(3), 129-139

CODEN: JPERFA; ISSN: 1397-002X

PUBLISHER: Blackwell Munksgaard

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Partitioning of 153 di- to hexapeptides in an aqueous dextran-PEG two-phase system containing 0.15 M NaCl in 0.01 M sodium phosphate buffer, pH 7.4 was examined. The relative hydrophobicity of the peptides was estimated and expressed in equivalent nos. of methylene units. Anal. of the data shows that

the additivity principle applies for the relative hydrophobicity of up to hexapeptides. The relative hydrophobicities of Trp, Glu, and Asp residues in heterooligopeptides are noticeably different from those in corresponding homooligopeptides. The relative hydrophobicity of peptides can be calculated and used as a structural descriptor in quant. structure-activity relationship anal. The peptide bitterness threshold is shown to be quant. related to the peptide structure described as a combination of the relative hydrophobicity and lipophilicity (logD) of peptides.

IT 2047-13-4 25615-38-7 35978-98-4

50674-18-5 74863-12-0

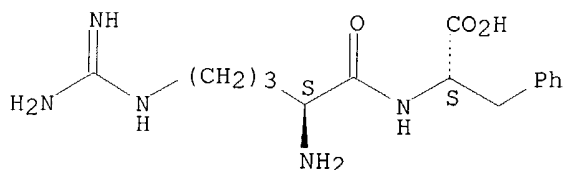
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(relative hydrophobicity of di- to hexapeptides as measured by aqueous two-phase partitioning)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

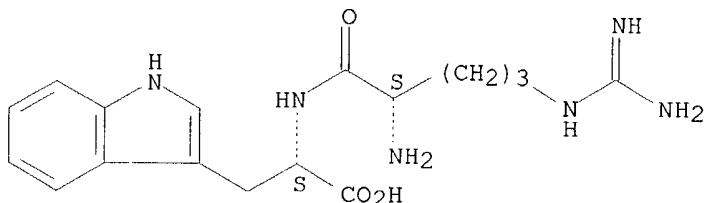
Absolute stereochemistry.



RN 25615-38-7 HCAPLUS

CN L-Tryptophan, L-arginyl- (9CI) (CA INDEX NAME)

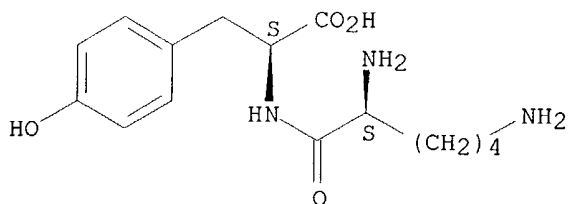
Absolute stereochemistry.



RN 35978-98-4 HCAPLUS

CN L-Tyrosine, L-lysyl- (9CI) (CA INDEX NAME)

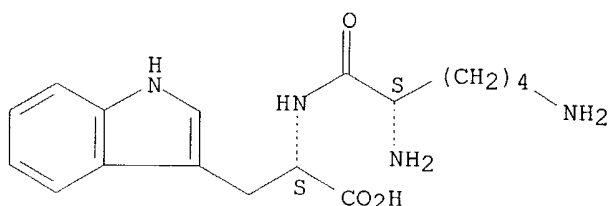
Absolute stereochemistry.



RN 50674-18-5 HCAPLUS

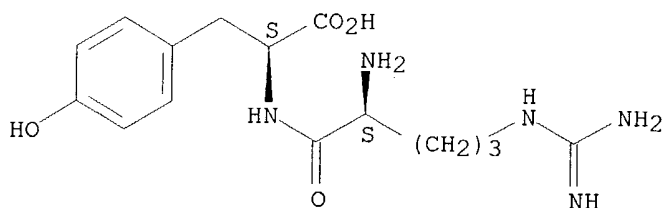
CN L-Tryptophan, L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 74863-12-0 HCAPLUS  
CN L-Tyrosine, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:41684 HCAPLUS

DOCUMENT NUMBER: 139:46402

TITLE: QSAR studies on dipeptides based on a combinatorial MHDV-GA-MLR method

AUTHOR(S): Liu, Shu-Shen; Yin, Chun-Sheng; Wang, Xiao-Dong; Wang, Lian-Sheng

CORPORATE SOURCE: State Key Laboratory of Pollution Control and Resources Reuse, Department of Environmental Science & Engineering, Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2002), 49(6), 1089-1096  
CODEN: JCCTAC; ISSN: 0009-4536

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A combinatorial method for estimating and predicting the biol. activities of two sets of dipeptides, a set of 48 compds. and another set of 58, was developed. The mol. holog. distance vector (MHDV) was employed to characterize the structures of the peptide mols. Preliminary selection of the MHDV descriptors was performed based on the number of the mols. having non-zero MHDV values. The final optimal descriptors were completed by a genetic algorithm-based variable selection procedure. Then the optimal descriptors are used to relate to the biol. activities of the peptides using the multiple linear regression (MLR) method. For two panels of dipeptides, the correlation coefficient of estns. are resp. 0.9651 for 48 peptides and 0.936 for 58 peptides, and the correlation coefficient of leave-one-out predictions are resp. 0.9452 and 0.9075.

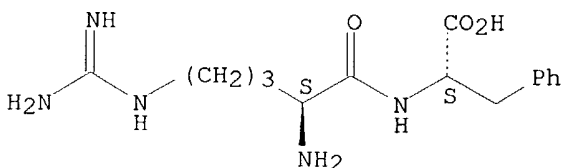
Searched by P. Ruppel

IT 2047-13-4 25615-38-7  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (QSAR studies on dipeptides based on a combinatorial MHDV-GA-MLR  
 method)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

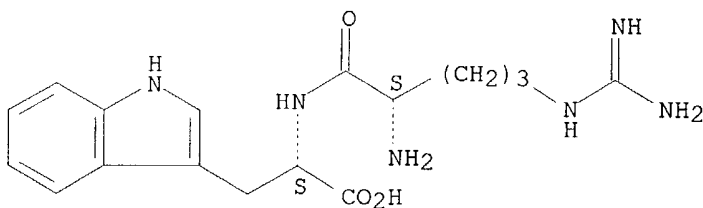
Absolute stereochemistry.



RN 25615-38-7 HCAPLUS

CN L-Tryptophan, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:814885 HCAPLUS

DOCUMENT NUMBER: 136:81581

TITLE: Molecular electronegativity-distance vector for  
 quantitative structure-activity relationship studies  
 of peptide analogues

AUTHOR(S): Liu, Yan; Liu, Shu-shen; Yin, Chun-sheng

CORPORATE SOURCE: College of Bioengineering, Chongqing University,  
 Chungking, 400044, Peop. Rep. China

SOURCE: Changde Shifan Xueyuan Xuebao, Ziran Kexueban (2001),  
 13(3), 44-52

CODEN: CDSYB4; ISSN: 1009-3818

PUBLISHER: Changde Shifan Xueyuan Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel mol. electronegativity-distance vector (MEDV) is proposed to  
 characterize the structures of peptide mols. containing heteroatoms such as N,  
 O, and S, unsatd. and conjugated chemical bonds such as C:O, C:C, and C:N  
 bonds and relate to biol. activities of two panels of dipeptides.  
 Utilizing multiple linear regression (MLR) method, two six-parameter  
 quant. structure-activity relationship (QSAR) models, one (labeled M1) for  
 a set of 58 dipeptides and another (M2) for 48 dipeptides, have been  
 developed with the correlation coefficient (R) of 0.842 3 for M1 and 0.819 9

for M2, and the root mean square error (RMS) of 0.535 for M1 and 0.357 for M2, between the estimated activities and the observed activities. To test the prediction ability of the QSAR models, a cross-validation procedure is performed by leave-one-out method with the predicted R of 0.790 6 for M1 and 0.742 2 for M2 and the predicted RMS of 0.608 (M1) and 0.417 (M2). The MEDV in the present paper only employs information about electronegativity of element atom type and length of chemical bond from the mol. graph and requires no 3D structures or mol. alignment or information related physicochem. properties. Besides, constructing QSAR model utilizes classical MLR technique and no principal component anal. (PCA) or partial least squares (PLS) method. So, the QSAR technique proposed in this paper is fast, easy to use, reproducible and predictable.

IT 2047-13-4 25615-38-7

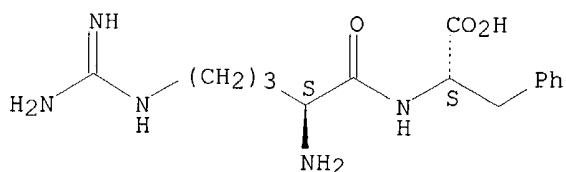
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(mol. electronegativity-distance vector for QSAR of dipeptides as inhibitors of angiotensin-converting enzyme)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

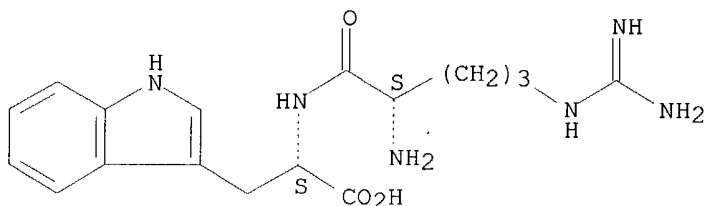
Absolute stereochemistry.



RN 25615-38-7 HCAPLUS

CN L-Tryptophan, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:15339 HCAPLUS

DOCUMENT NUMBER: 116:15339

TITLE: Minimum analog peptide sets (MAPS) for quantitative structure-activity relationships

AUTHOR(S): Hellberg, Sven; Eriksson, Lennart; Jonsson, Joergen; Lindgren, Fredrik; Sjoestroem, Michael; Skagerberg, Bert; Wold, Svante; Andrews, Peter

CORPORATE SOURCE: Dep. Chem., Univ. Umea, Umea, S-90187, Swed.

SOURCE: International Journal of Peptide & Protein Research (1991), 37(5), 414-24

Searched by P. Ruppel

CODEN: IJPPC3; ISSN: 0367-8377  
DOCUMENT TYPE: Journal  
LANGUAGE: English

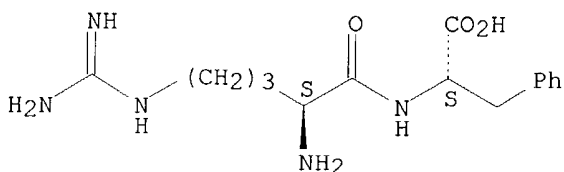
AB The previously published peptide sets were compared with smaller sets of peptides selected according to statistical designs. Min. analog peptide sets (MAPS) constructed by factorial or fractional factorial designs in physicochem. properties contained substantial structure-activity information. Although five to six times smaller than the originally published peptide sets, the MAPS resulted in QSAR models able to predict biol. activity. The QSARs derived from a MAPS of 9 dipeptides and from 58 dipeptides inhibiting angiotensin-converting enzyme were of equal strength. For a set of bitter tasting dipeptides, an incomplete MAPS of 10 dipeptides gave just as good a model as the model based on a set of 48 dipeptides. Other non-designed sets of peptides gave QSARs with poor predictive power. MAPS centered on a lead peptide can be constructed to explore specifically the physicochem. and biol. properties in the vicinity of the lead. Small information-rich peptide sets MAPS can be constructed on the basis of statistical designs with principal properties of amino acids as design variables.

IT 2047-13-4 25615-38-7  
RL: BIOL (Biological study)  
(angiotensin-converting enzyme inhibition by, min. analog set technique for structure design in relation to)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

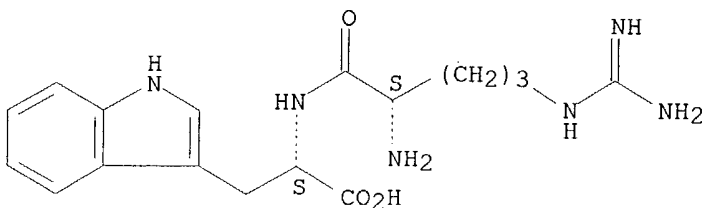
Absolute stereochemistry.



RN 25615-38-7 HCAPLUS

CN L-Tryptophan, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:435778 HCAPLUS

DOCUMENT NUMBER: 109:35778

TITLE: Studies on **flavored** peptides. Part V. A mechanism for bitter **taste** sensibility in peptides

AUTHOR(S): Ishibashi, Norio; Kouge, Katsushige; Shinoda, Ichizo;



CORPORATE SOURCE: Kanehisa, Hidenori; Okai, Hideo  
SOURCE: Fac. Eng., Hiroshima Univ., Shitami, Japan  
Agricultural and Biological Chemistry (1988), 52(3),  
819-27

DOCUMENT TYPE: CODEN: ABCHA6; ISSN: 0002-1369

LANGUAGE: Journal

LANGUAGE: English

AB To estimate the steric distance between the bitter taste determinant sites in peptides, some cyclic dipeptides, amino acid anilides, amino acid cyclohexylamides, and benzoyl amino acids were synthesized and their tastes were evaluated. The diketopiperazine ring of cyclic dipeptides acted as a bitter taste determinant site due to its hydrophobicity. The steric distance between 2 sites was estimated as 4.1 Å from the mol. models of cyclic dipeptides composed of typical amino acids in the bitter peptides. Due to the hypothesis of 2 bitter taste determinant sites, which bind with the bitter taste receptor via a binding unit and a stimulating unit, a mechanism for the bitterness in peptides was postulated.

IT 2047-13-4P

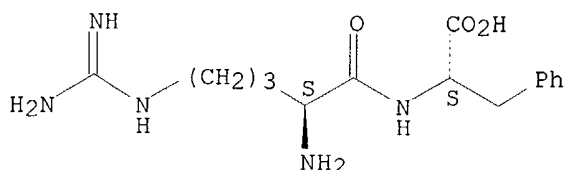
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and **taste** to human of)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:72843 HCAPLUS

DOCUMENT NUMBER: 108:72843

TITLE: Studies on **flavored** peptides. Part II.  
Bitterness of phenylalanine- and tyrosine-containing peptides

AUTHOR(S): Ishibashi, Norio; Sadamori, Koji; Yamamoto, Osamu;  
Kanehisa, Hidenori; Kouge, Katsushige; Kikuchi,  
Eiichi; Okai, Hideo; Fukui, Sakuzo

CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashi-Hiroshima, 724,  
Japan

SOURCE: Agricultural and Biological Chemistry (1987), 51(12),  
3309-13

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To investigate the role of phenylalanine and tyrosine residues in the bitter taste of peptides, some oligopeptides containing phenylalanine or tyrosine were synthesized and their taste was evaluated. The hydrophobicity of the phenylalanine or tyrosine mol. caused the marked bitter taste in peptides. The bitterness was more intense when

phenylalanine was located at the C-terminus and when the content of phenylalanine or tyrosine was increased in peptides. The hydrophobic residue in peptides functioned as a bitter taste determinant site. The exptl. results suggest the existence of an addnl. site for the bitter taste of peptides.

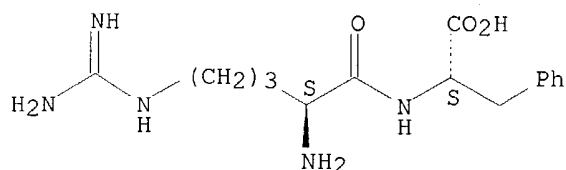
IT 2047-13-4 6235-35-4, Lys-Phe

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
(bitterness of, to human, structure in relation to)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

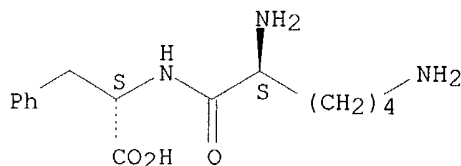
Absolute stereochemistry.



RN 6235-35-4 HCAPLUS

CN L-Phenylalanine, L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:593890 HCAPLUS

DOCUMENT NUMBER: 103:193890

TITLE: Studies on a model of bitter peptides including arginine, proline, and phenylalanine residues

AUTHOR(S): Nosho, Yasuharu; Shinoda, Ichizo; Otagiri, Ken; Okai, Hideo

CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashi-Hiroshima, 724, Japan

SOURCE: Peptide Chemistry (1985), Volume Date 1984, 22nd, 323-8

CODEN: PECHDP; ISSN: 0388-3698

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Bitter peptides contained either hydrophobic amino acids, or arginine and(or) proline. Peptides containing only arginine, proline, and phenylalanine were prepared and tested for bitterness. Bitterness generally increased with increasing nos. of amino acids. Arg-Arg-Pro-Pro-Phe-Phe-Phe was 500-fold as bitter as caffeine and 1/2 as bitter as brucine (the most bitter known substance), and is thus the most bitter peptide found so far. Differences in bitterness were also observed when L-phenylalanine or D-phenylalanine were used.

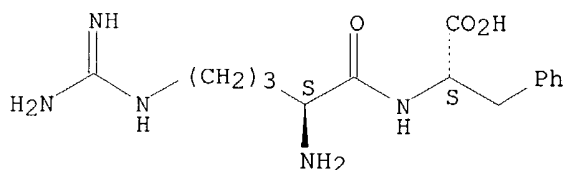
IT 2047-13-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(bitterness of)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:405112 HCAPLUS

DOCUMENT NUMBER: 103:5112

TITLE: Studies on a model of bitter peptides including arginine, proline and phenylalanine residues. I. Bitter **taste** of di- and tripeptides, and bitterness increase of the model peptides by extension of the peptide chain

AUTHOR(S): Otagiri, Ken; Noshio, Yasuharu; Shinoda, Ichizo; Fukui, Hiroshi; Okai, Hideo

CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Shitami, Higashi-Hiroshima, 724, Japan

SOURCE: Agricultural and Biological Chemistry (1985), 49(4), 1019-26

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To elucidate the relation between bitter taste and chemical structure in peptides, various kinds of model bitter peptides containing arginine, proline and phenylalanine were synthesized, and the contribution of the individual amino acids to the bitter taste was examined. To strengthen the bitterness in di- and tripeptides, the hydrophobic amino acid had to be located at the C-terminal and, conversely, the basic amino acid should be located at the N-terminal. Further, a strong bitter taste was observed when arginine was contiguous to proline such as Arg-Pro [2418-69-1], Gly-Arg-Pro [96817-13-9] and Arg-Pro-Gly [96817-14-0]. A synergistic effect for bitter taste was observed in the peptides whose structure is (Arg)<sub>1</sub>-(Pro)<sub>m</sub>-(Phe)<sub>n</sub> (1 = 1, 2; m, n = 1-3) by increasing the number of amino acids. Among them the octapeptide (Arg-Arg-Pro-Pro-Pro-Phe-Phe-Phe [96817-15-1]) possessed an extremely bitter taste with its threshold value of 0.002 mM and was the most bitter among the peptides.

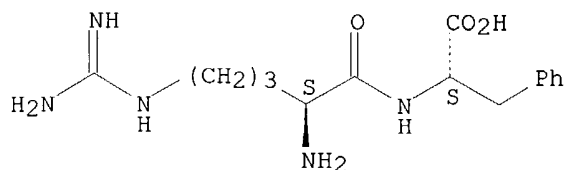
IT 2047-13-4

RL: PRP (Properties)  
(bitterness of, mol. structure in relation to)

RN 2047-13-4 HCAPLUS

CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

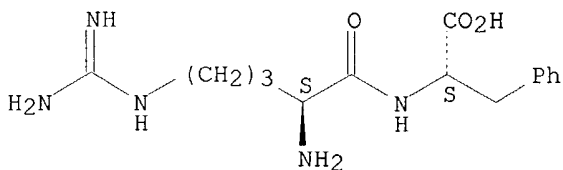


L14 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1980:526374 HCAPLUS  
 DOCUMENT NUMBER: 93:126374  
 TITLE: Relationship between bitterness and chemical structure of cyclic dipeptides  
 AUTHOR(S): Kouge, Katsushige; Kanehisa, Hidenori; Okai, Hideo; Oka, Satoru  
 CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Hiroshima, 730, Japan  
 SOURCE: Peptide Chemistry (1979), Volume Date 1978, 16th, 105-8  
 CODEN: PECHDP; ISSN: 0388-3698  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Eighteen cyclic dipeptides were synthesized, and the bitterness of these compds. was tested organoleptically by panel evaluation. All of the cyclic dipeptides tested were more bitter than the corresponding linear dipeptides. Among the 11 hydrophobic amino acid-containing cyclic dipeptides, the bitterness increased with increasing hydrophobicity. The 4 cyclic dipeptides containing proline, arginine, and phenylalanine, which are typical constituents of bitter peptides, all had strong bitter taste, except for cyclo-(Pro-Pro) [19943-27-2]. There was some variation in bitterness with the amino acid sequence of these cyclid dipeptides. From the above results, the diketopiperazine [106-57-0] ring itself is necessary for the intense bitterness of the cyclic dipeptides and is involved in the mechanism of bitter taste proposed by H. Okai (1977).

IT **2047-13-4**  
 RL: PRP (Properties)  
 (bitterness of)  
 RN 2047-13-4 HCAPLUS  
 CN L-Phenylalanine, L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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=&gt; b hcaplus

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FILE COVERS 1907 - 19 Nov 2004 VOL 141 ISS 22

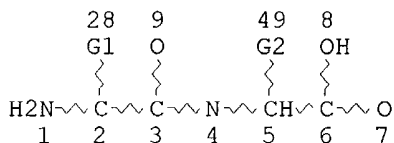
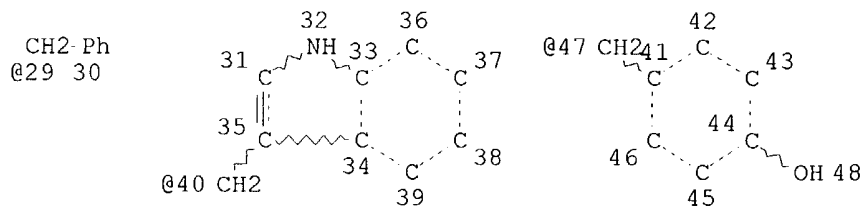
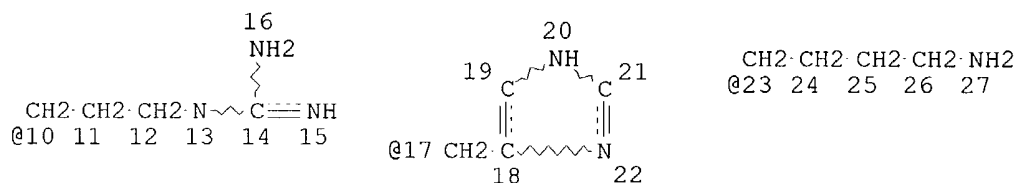
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L8 STR



VAR G1=10/17/23

VAR G2=29/40/47

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 7

CONNECT IS E1 RC AT 9

Searched by P. Ruppel

CONNECT IS X2 RC AT 19  
 CONNECT IS X2 RC AT 21  
 CONNECT IS X2 RC AT 31  
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 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 49

## STEREO ATTRIBUTES: NONE

L26 77 SEA FILE=REGISTRY SSS FUL L8

L27 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L26 AND MAILLARD/BI

=&gt; d all 127

L27 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:259690 HCAPLUS

DN 138:270653

ED Entered STN: 04 Apr 2003

TI Flavor-active peptides from cocoa beans

IN Kochhar, Sunil; Hansen, Carl Erik; Juillerat, Marcel Alexandre

PA Societe Des Produits Nestle S.A., Switz.

SO Eur. Pat. Appl., 14 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM A23L001-035

ICS A23G001-00

CC 17-6 (Food and Feed Chemistry)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1297753	A1	20030402	EP 2001-123585	20011001
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	WO 2003028479	A1	20030410	WO 2002-EP10031	20020906
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004224077	A1	20041111	US 2004-812088	20040330
PRAI	EP 2001-123585	A	20011001		

WO 2002-EP10031 A1 20020906

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 1297753	ICM	A23L001-035
	ICS	A23G001-00
EP 1297753	ECLA	A23G001/00K; A23G003/00K; A23L001/227K; A23L001/231; A23L001/234

AB The present invention pertains to specific peptides obtainable from cocoa beans and giving rise to a particular and distinct flavor when subjected to a **Maillard** reaction with reducing sugars. In particular the present invention pertains to the use of said specific peptides for the preparation of a chocolate flavor, specifically a cocoa and a caramel flavor, a floral or specifically, a bonbon flavor, a bready flavor, a roasted flavor and a meat flavor.

ST flavor food cocoa bean peptide **Maillard** product

IT Cocoa products  
(beans; flavor-active peptides from cocoa beans)

IT Beverages  
Caramel (color)  
Chocolate  
Flavor  
Flavoring materials  
Ice cream  
Milk  
Puddings  
(flavor-active peptides from cocoa beans)

IT **Maillard** reaction products  
Peptides, biological studies  
RL: BSU (Biological study, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(flavor-active peptides from cocoa beans)

IT Bread  
Chocolate  
Cocoa products  
(flavor; flavor-active peptides from cocoa beans)

IT Food  
(infant; flavor-active peptides from cocoa beans)

IT Flavoring materials  
(meat flavors; flavor-active peptides from cocoa beans)

IT Feed  
(pet; flavor-active peptides from cocoa beans)

IT Food  
(prepared; flavor-active peptides from cocoa beans)

IT Carbohydrates, biological studies  
RL: FFD (Food or feed use); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)  
(reducing sugars; flavor-active peptides from cocoa beans)

IT Milk preparations  
(yogurt; flavor-active peptides from cocoa beans)

IT 50-99-7, Dextrose, biological studies 57-48-7, D-Fructose, biological studies 58-86-6, D-Xylose, biological studies 59-23-4, D-Galactose, biological studies 63-42-3, Lactose 69-79-4, Maltose 634-74-2, D-Rhamnose 730-08-5 **2047-13-4** 3061-88-9 3061-90-3 3061-91-4 3303-31-9 3615-37-0, D-Fucose 3617-45-6 3918-87-4 3918-92-1 **6235-35-4**, Lys-Phe 10323-20-3, D-Arabinose 13187-90-1 13433-02-8 13589-04-3 17355-09-8 20727-65-5

21064-18-6 22677-62-9 24046-71-7 27493-61-4 45234-02-4  
50299-12-2 52899-09-9

RL: FFD (Food or feed use); RCT (Reactant); BIOL (Biological study); RACT  
(Reactant or reagent); USES (Uses)  
(flavor-active peptides from cocoa beans)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

(1) Nestle Sa; EP 1008305 A 2000 HCAPLUS

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